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13. ABSTRACT *(Maximum 200 Words)*

Various internal variable theories for materials undergoing phase transformation have been developed. Specific topics include the relaxation phenomena in shape-memory alloys, domain patterns in ferroelectrics, the effect of texture on the shape-memory effect in polycrystals, the failure of ceramics and martensitic thin films.

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List Co-PIs/Subcontractors, if any

None

ACCOMPLISHMENTS/NEW FINDINGS

1. Various relaxation processes adversely affect the performance of shape-memory alloys. Though much is known experimentally, there is no concensus on the mechanism and various questions remain open. The one-dimensional phenomenological, but predictive, model developed by the PI with R. D. James and P. J. Swart will provide a useful tool to predict the behavior of such alloys. We have explored this model numerically and our mathematical analysis has provided some suprising insights into "hybrid" dynamical systems. The PI and M. Jabbour have extended this model to three dimensions. This model will be useful not only in shape-memory alloys, but also in materials where ordering is accompanied with significant strain.

2. Ferroelectric ceramics are commonly used as actuator materials. However, the strain they provide is very small. The current research of Y.C. Shu and the PI explores whether (a) texturing the ceramic and (b) a combination of applied mechanical load and electric field will lead to significant improvement. We have completed our study of single crystals and have proposed an actuator configuration which should provide strains as large as 1%.

3. The PI and Y.C. Shu have developed a model and used it to show that texture is a crucial factor in determining the shape-memory effect in polycrystals. In particular, it is established that texture is the reason why the strains recoverable in Ti-Ni are so much larger than those in Cu-based shape-memory alloys in rolled, extruded or drawn specimens. Further, it is shown that both these materials recover relatively small strains in sputter-deposited thin films due to unfavorable texture. These results are in good agreement with experimental observations. Finally, the model is used to suggest textures for imporved shape-memory effect.

4. Confined heterogeneous brittle solids loaded under far-field uniaxial compression are often observed to split along the loading axis. We have developed a theory which accords this phenomenon an energetic interpretation: the solid splits because in so doing it reduces its total energy, defined as the sum of bulk strain energy and surface energy. The heterogeneous microstructure gives rise to a complex stress distribution in the intact solid. We show that the change in energy due to the release of the microstructural stresses may exceed the cost in fracture

energy. Critical conditions for splitting are formulated for polycrystalline solids as a function of readily measurable material properties and applied stresses. The predictions of the theory are found to be in remarkably good agreement with experimental observations in ceramics and rocks.

5. Shape-memory alloys have the largest energy output per unit volume per cycle of known actuator systems, and their frequency response is not limited in thin films. Hence, shape-memory alloys are ideal actuator materials in micromachines. The heart of the shape-memory effect lies in a martensitic phase transformation and the resulting microstructure. It is wellknown that microstructure can be significantly different in thin films as compared to bulk materials. We have developed an internal variable theory which is valid for single crystal martensitic thin films. We show that single crystal films of shape memory material offer interesting possibilities for producing very large deformations at small scales. In addition, from a mathematical point of view, the derivation of the internal variable theory is one of the first rigourous derivations of membrane theories and also provides a possible method to derive plate and shell theories.

PERSONNEL SUPPORTED

Faculty
None

Post-Docs
None

Graduate Students
Yi-Chung Shu
Michel Jabbour

Other (please list role)
None

PUBLICATIONS

APPEARED/ACCEPTED

Books/Book Chapters

K. Bhattacharya, "A theory of martensitic microstructure and its implications on the shape-memory effect," to appear in "Shape Memory Alloys" (ed. G. Airoldi, S. Miyazaki and I. Müller), Trans. Tech. Publications (1998).

Journals

K. Bhattacharya, R.D. James and P.J. Swart, "Relaxation in shape-memory alloys. Part I: Mechanical Model", *Acta Materialia* 45 (1997), 4547-4560.

K. Bhattacharya, R.D. James and P.J. Swart, "Relaxation in shape-memory alloys. Part II: Thermomechanical Model and Proposed Experiments", *Acta Materialia* 45 (1997), 4561-4568.

N. Simha and K. Bhattacharya, "Equilibrium conditions at corners and edges of an interface in a multiphase solid", *Mat. Sci. Engng. A* 238 (1997), 32-41.

K. Bhattacharya, M. Ortiz and G. Ravichandran, "An energy-based model of compressive failure in inhomogeneous brittle solids", to appear in *J. Mech. Phys Solids* (1998).

N. Simha and K. Bhattacharya, "Kinetics of phase boundaries with edges and junctions", to appear in *J. Mech. Phys Solids* (1998).

K. Bhattacharya and R.D. James, "A theory of thin films of martensitic materials with applications to microactuators", to appear in *J. Mech. Phys. Solids* (1998).

K. Bhattacharya, R.V. Kohn and S. Kozlov, "Some examples of nonlinear homogenization involving nearly degenerate energies", to appear in *Proc. Royal Soc. London A* (1998).

Conferences

K. Bhattacharya and R.V. Kohn, "Recoverable Strain in Shape-memory Polycrystals", Proceedings of ICOMAT-95, *J. de Phys. III*, vol. 5 (1996), Colloque C8, pp. 261-266.

K. Bhattacharya and R.D. James, "A theory of shape-memory thin films with applications" in "Active Materials Systems", *Mat. Res. Soc.* Vol. 459, 311-316 (1997).

K. Bhattacharya, R.V. Kohn and Y.C. Shu, "The Taylor estimate of recoverable strains in shape-memory polycrystals", to appear in the *IUTAM Symp. on Trans. Problems in Composite and Active Materials* (ed. Bahei-El-Din, Y.A. and Dvorak, G.J.), Kluwer to appear (1998).

K. Bhattacharya, "Energy minimization and nonlinear problems in polycrystalline solids" in "Computer aided design of high temperature materials (ed. A. Pechenick, R. Kalia, P. Vaishista), Oxford University Press, to appear (1998).

SUBMITTED

Books/Book Chapters
None

Journals

Y.C. Shu and K. Bhattacharya, "The influence of texture on the shape-memory effect in polycrystals" submitted to *Acta Materialia*(1998).

K. Bhattacharya, "Crystallographic attributes of a shape-memory alloy", submitted to *ASME J. Engng. Mat. Tech.* (1998).

K. Bhattacharya, B. Li and M. Luskin, "The simply laminated microstructure in martensitic crystals undergoing a cubic to orthorhombic phase transformation", submitted to *Arch. Rat. Mech. Anal.* (1998).

Conferences
None

DRAFT

Books/Book Chapters
None

Journals

Y.C. Shu and K. Bhattacharya, "Domain patterns and macroscopic behavior of ferroelectric materials" (1998).

Y.C. Shu, "Heterogeneous thin films of martensitic materials" (1998).

K. Bhattacharya, R.D. James and P.J. Swart, "Analysis of a nonlinear dynamic model of shift relazation in Au-47.5% Cd and related materials", to be submitted to *J. of Nonlinear Science* (1998)

Conferences
None

INTERACTIONS/TRANSITIONS

The PI attended and presented papers at the following conferences:

Martensite Workshop, Northwestern University, Evanston, June 1995.

International Conference on Martensitic Transformations (ICOMAT-95), Lausanne, Switzerland, August, 1995.

IMA workshop on "Phase Transformations, Composite Materials and Microstructures," Institute for Mathematics and Its Applications, Minneapolis, September 18-22, 1995. Also spent three weeks in residence at the IMA during September 1995.

Symposium on the "Mathematics of Thermodynamically Driven Microstructure," TMS/ASM Materials Week, October - November, 1995.

SPIE 1996 Symposium on Smart Structures and Materials, San Diego, February, 1996.

ASME Mechanics and Materials Conference, Baltimore, June, 1996.

Symposium on Thermodynamische Materialtheorien at the Mathematisches Forschungsinstitut Oberwolfach, Germany, September 1996.

Applied Mathematics Workshop for Materials Studies and Industrial Applications, Pennsylvania State Univ., State College, October 1996.

IUTAM Symposium on Transformation problems in composite and active materials, Cairo, Egypt, March 1997.

Second SIAM conference on Mathematical Aspects of Materials Science, Philadelphia, May 1997 (Plenary Talk).

Computer Aided Design of High Temperature Materials, Santa Fe, July 1997.

The PI attented:

16th Annual International Conference of the Center for Nonlinear Studies, Los Alamos National Laboratory, May 13-17, 1996.

Consultative And Advisory Functions To Other Laboratories And Agencies

None

Transitions

None

NEW DISCOVERIES, INVENTIONS, OR PATENT DISCLOSURES

None

HONORS/AWARDS

The PI has been awarded the Charles Lee Powell Award 1997 by the Division of Engineering and Applied Science, California Institute of Technology.